

2020 DOE Vehicle Technologies Office Annual Merit Review

# Multiscale Development and Validation of the Stainless Steel Alloy Corrosion (SStAC) Tool for High Temperature Engine Materials

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POWERING THE NEW ENGINEER TO TRANSFORM THE FUTURE

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#### Overview

#### **Timeline**

- Project start date: Oct 1, 2018
- Project end date: Dec 31, 2021
- Percent complete: 45%

#### **Budget**

- Total project funding
  - DOE Share: \$1500K
  - Cost Share: \$375K
- DOE funding for FY2020: \$500K
- DOE funding for FY 2021: \$500K

#### Barriers

- Corrosion sensitization of valve steels at high temperature
- Lack of predictive modeling mandates conservative design

#### **Partners**









#### Relevance

#### **Barrier**

 Conservative design is mandated by a lack of predictive modeling of the sensitization of stainless steels to corrosion at high temperature



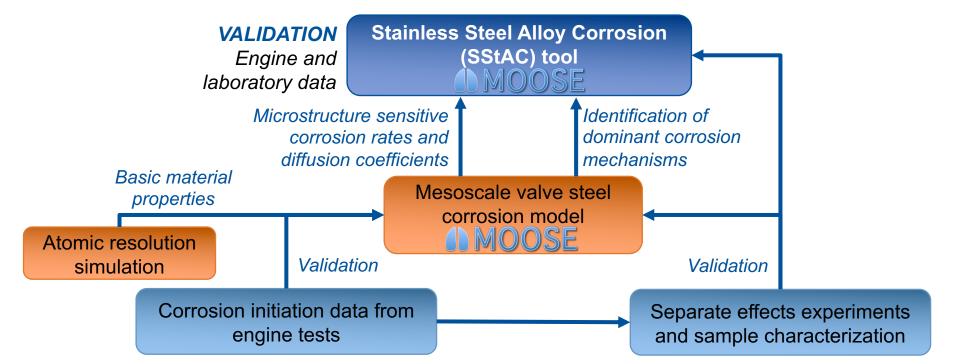
#### **Objectives**

- Develop the open source Stainless Steel Alloy Corrosion (SStAC) tool for modeling corrosion of 21-2N, 21-4N, and 23-8N valve steels in an engine environment.
- Quantify the impact of microstructure and alloy composition on valve steel corrosion using laboratory and engine experiments and mesoscale modeling and simulation.



### Approach:

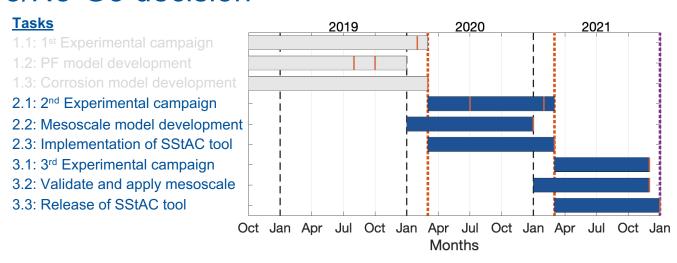
The SStAC tool will be developed using a multiscale approach validated by laboratory and engine data





#### Milestones:

# We have completed our first three tasks and achieved our first Go/No-Go decision



- BP1 Go-No Go: Corrosion model must be within 25% of experimental data
- BP2 Go-No Go: SStAC tool must function in 1D, 2D, and 3D
- BP3 Go-No Go: Final SStAC tool must predict corrosion rate with < 10% error



# Technical Accomplishments and Progress: Overall Accomplishments

### nanometers Atomic-Scale Simulations

 We have begun to determine critical alloy properties

### 100's of microns Mesoscale Simulations

 We have completed the basic electrochemical phase field corrosion model

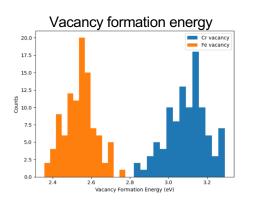
# microns to millimeters Lab experiments

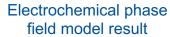
We have completed the first experimental campaign

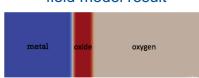
#### millimeters and up Engineering scale

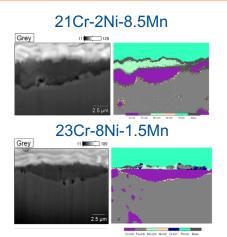
 The initial corrosion model meets our accuracy requirement

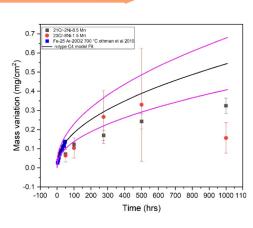
#### Specific properties and models are determined and passed up the scale





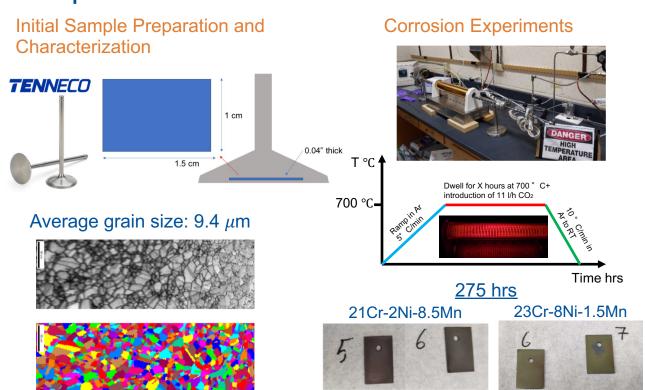




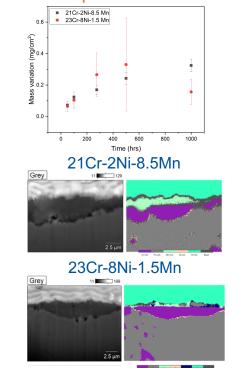




# Technical Accomplishments and Progress: Experiments



#### Final sample characterization

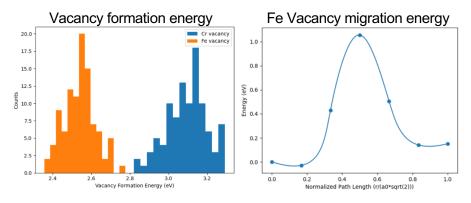




# Technical Accomplishments and Progress: Atomic and Mesoscale Simulation

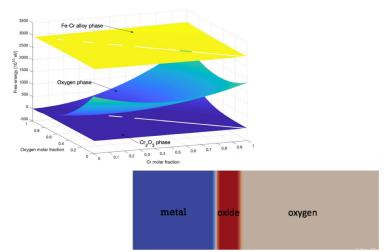
#### Atomic-scale simulations

- Density functional theory (DFT) and molecular dynamics (MD) provide missing material properties
- We are investigating two embedded atom MD potentials (Zhou and Bonny)



#### Mesoscale model

- We are developing a quantitative phase field model of corrosion in Fe-Cr-Mn alloys
  - We are focusing on Cr and Mn oxide formation
  - We have included the impact of electrochemistry





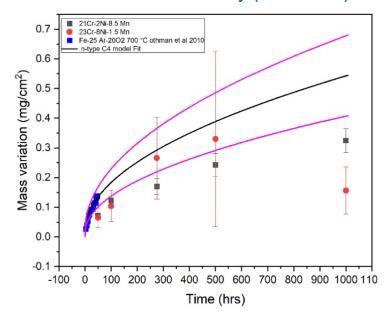
# Technical Accomplishments and Progress: Engineering Scale Model Development

#### Corrosion model summary

- The corrosion model uses the Coupled Current Charge Compensation (C4) method
- Primary assumptions
  - Defect fluxes are constant throughout the oxide layer
  - Interfacial reactions are at equilibrium
  - Zero net charge throughout the oxide
- Calibrated parameters
  - Oxygen vacancy migration energy
  - Electron untrapping energy
- Model was calibrated using literature data

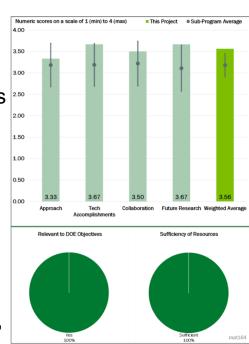
#### Corrosion model results

 Calibrated model is within 25% of the error bars for the 23Cr-8Ni-1.5 Mn alloy (Go/No-Go)



### Response to previous year reviewers' comments

- The results obtained from the unique corrosion apparatus may not compare with industry standards
  - The apparatus was developed and verified using ASTM standards
- Explain how the PI coordinates activities across the country
  - We hold monthly project meetings and a yearly onsite meeting
- Is the cost-share from the industry partner absent?
  - Cost-share is met by TENNECO and UF
- Reliable material properties for the SStAC tool are critical. It will be ideal if experiments are used to calibrate them.
  - We are obtaining material properties from new experimental data, literature data, and lower length-scale simulation





#### Collaboration and Coordination with Other Institutions



Developing macroscale SStAC tool, carrying out laboratory corrosion experiments and analyzing corroded samples



Providing mentorship and guidance on the application and development of the Multiphysics Object-Oriented Simulation Environment (MOOSE)

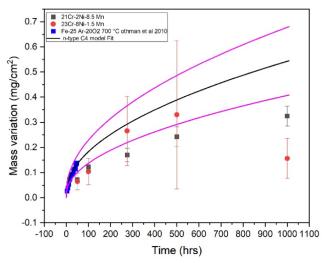


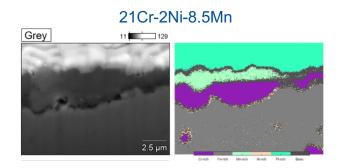
Providing engine valve material, sample preparation, sample characterization, and carrying out engine testing

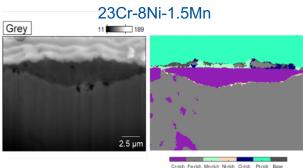


### Remaining challenges and barriers

- The corrosion model currently does not consider alloying elements nor the material microstructure
- We don't know the impact of temperature cycling and combustion gas composition on the corrosion behavior
- The corrosion model needs to be implemented in a finite element model





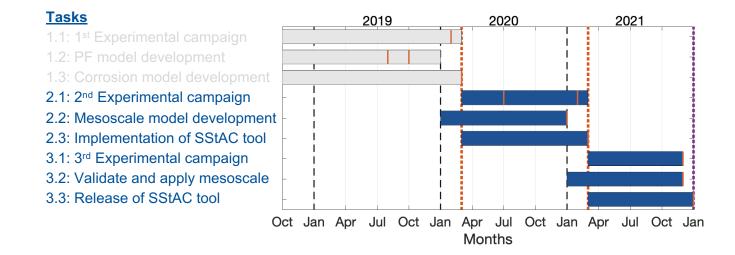


# Proposed Future Research (subject to change based on funding levels)

- Ongoing (FY 2020)
  - Samples will be corroded after thermal annealing. Engine tests will also be carried out.
  - The phase field model will be coupled with mechanics. DFT and MD simulations will be used to calculate more properties.
  - The SStAC tool will be implemented in MOOSE. The numerical capability of the corrosion tool will be evaluated; **Go/No-Go**.
- Future (FY 2021)
  - Samples will be characterized and tests will be carried out with thermal cycling
  - The mesoscale model will be completed using data from the DFT and MD simulations, and it will be used to quantify the impact of microstructure on corrosion
  - The SStAC tool will be completed and validated against data from the literature, from Federal-Mogul, and from the project. **End-of-project goal**.

### Summary

- The Stainless Steel Alloy Corrosion (SStAC) tool will
  - Be open-source, based on the MOOSE framework
  - Include impact of microstructure and alloying elements from lower length-scale simulations
  - Be validated using new data from laboratory and engine experiments



# Herbert Wertheim College of Engineering UNIVERSITY of FLORIDA